On the calculation of single ion activity coefficients in homogeneous ionic systems by application of the grand canonical ensemble - DTU Orbit (11/12/2018)

The grand canonical ensemble has been used to study the evaluation of single ion activity coefficients in homogeneous ionic fluids. In this work, the Coulombic interactions are truncated according to the minimum image approximation, and the ions are assumed to be placed in a structureless, homogeneous dielectric continuum. Grand canonical ensemble Monte Carlo calculation results for two primitive model electrolyte solutions are presented. Also, a formula involving the second moments of the total correlation functions is derived from fluctuation theory, which applies for the derivatives of the individual ionic activity coefficients with respect to the total ionic concentration. This formula has previously been proposed on the basis of somewhat different considerations.

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